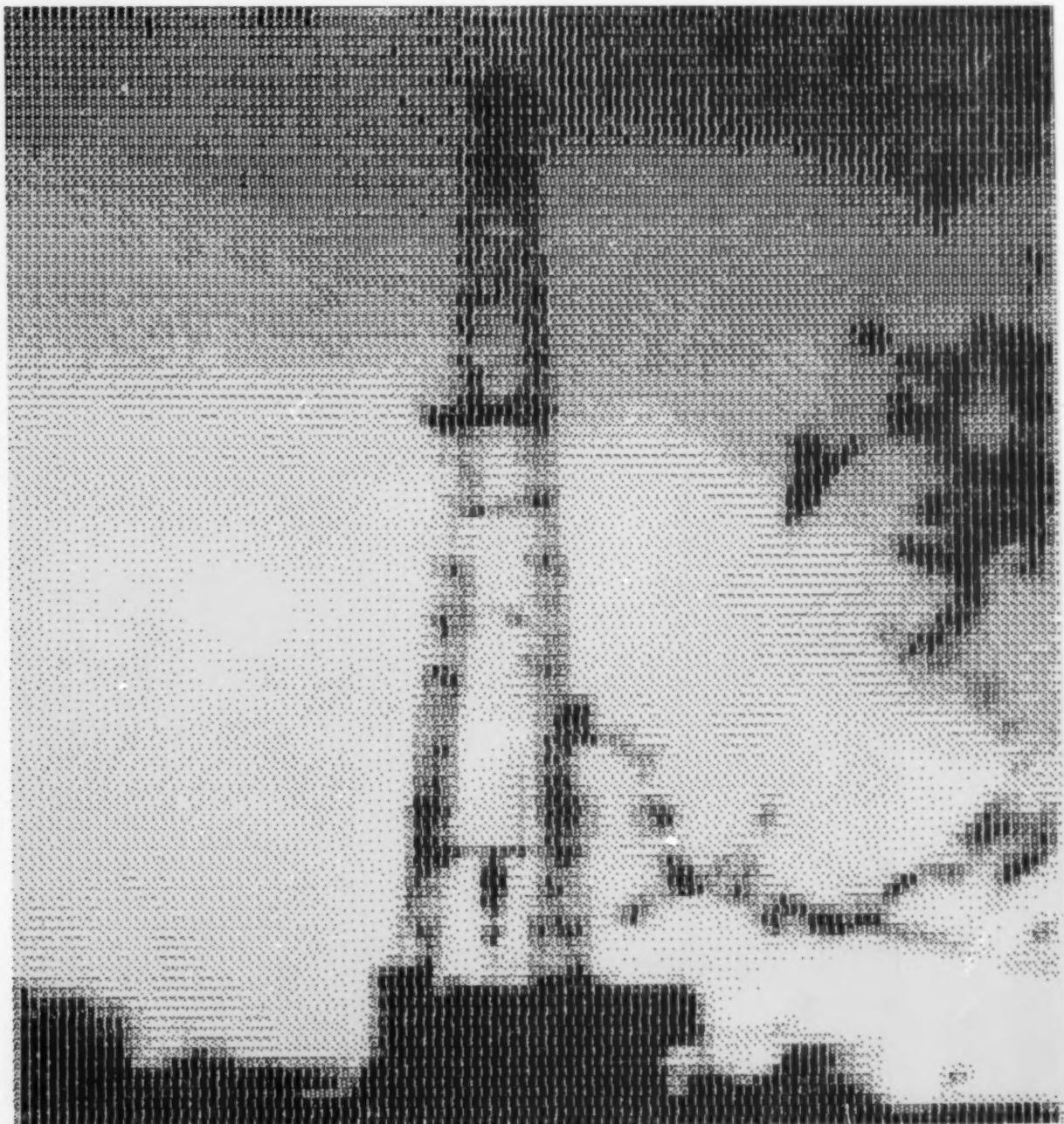


DIMENSIONS

NBS

The magazine of the
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of Standards
U.S. Department
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January/February 1980



EASTERN MICHIGAN UNIVERSITY

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ENERGY FORECASTING. See page 8.

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COMMENT

APPLIED MATHEMATICS AT NBS



tions, but few are aware of the day-to-day mathematical supporting services that are provided for all NBS programs and staff.

The subject areas of mathematical and computing sciences are vast, rapidly developing, and very active in a research sense. This rapid evolution, spurred by developments in computing technology, has had an obvious impact on the applications of mathematics in the programs of NBS.

The quality and integrity of NBS experiments and data depend in a fundamental fashion on the mathematical, statistical, and computing methods used throughout the experimental process. The design and adaptive control of NBS laboratory procedures, the development and validation of measurement and calibration systems, the automated acquisition and correct analysis of experimental data—these and other basic operations all depend upon mathematics and computing for their accomplishment.

The use and refinement of sophisticated theories, the application of analytical methods, the evolution from linear physical theories to present day non-linear developments, and much of NBS research in the physical and engineering sciences place heavy demands upon mathematical and computer techniques.

The mathematical modeling and analysis of complex systems, the solution of many applied problems, and the accurate and efficient computation of numerical results of all kinds employ mathematical methods from analysis, computer science, statistics, and operations research, of both traditional and developmental character.

The work of applied mathematicians is seldom directly visible to the technical public served by the National Bureau of Standards. Many scientists are familiar with the widely used NBS *Handbook of Mathematical Functions*,

Applications of mathematical developments are seen in:

—composition of alloy-physics phase diagrams, with the help of a *data management system* and *interactive graphics* to display the underlying experimental relations.

—achieving methods of designing fire-safe health-care facilities for minimum cost, by the use of *linear programming* for the basis of the Fire Safety Evaluation work sheet.

—determining the variation effects in atomic clock intercomparisons via the propagation of LORAN-C signals, by means of *time-series analysis*.

—modeling the evacuation of building occupants by *network flow optimization*—this technique permits designers to explore the consequences of changes in building design for best possible time-of-evacuation.

—rapid updating of orbit calculations for time-signal satellites, through an algebraic expansion obtained by automated *symbol manipulation*.

—improvement of manufacturer-supplied FORTRAN routines for minicomputers, via *validation algorithms* for superprecision functions.

The NBS program in the mathematical sciences, which includes mathematics, applied mathematics, operations research, statistics, and computer science, continues to provide general-purpose methods and expert consultation or collaboration to promote the use of the best available mathematical and computational techniques.

A handwritten signature in cursive script that reads "B. H. Colvin".

Burton H. Colvin
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Contents

ARTICLES

- 2** **Equity Beyond the Marketplace**
Meeting New Challenges Through SRM's
- 8** **Energy Forecasting: Improving on the Crystal Ball**
Models, Computers, and Fuel Supplies
- 13** **In the Pursuit of Precision**
NBS Grants for Research on Fundamental Constants

INTERFACE

- 16** **ON LINE WITH INDUSTRY**
NBS Measurement Seminars
- 17** **STANDARD STATUS**
Gas SRM's for Emissions Testing of Heavy Duty Vehicles
- 18** **STAFF REPORTS**
Eddy Current Imaging System
Economical and Accurate Method for Calculation of Atomic Properties
Resolution of Photon-Recoil Components of Visible Spectral Line

UPDATE

- 21** **CONFERENCES**
Workshop on Computer Interface Standards
Computer Network Protocols Symposium
Conference Calendar
- 22** **PUBLICATIONS**
Building Technology Publications Catalog
Stability of (Thin Film) Solar Cells and Materials
Slide Programs for Architects on Noise, Windows
Computer Program Documenting Practices, Criteria
NBS Publications
- 24** **NEWS BRIEFS**

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Equity Beyond the Marketplace

by Donald R. Johnson



This text has been edited from the keynote address of Dr. Donald R. Johnson, Deputy Director for Programs of NBS' National Measurement Laboratory, to the National Conference on Weights and Measures (NCWM), July 1979. NCWM, established in 1905 by the first NBS director, is an annual forum for State and local weights and measures officials and NBS representatives. Participants develop policies and model regulations to assure equity in the marketplace.

EQUITY in the marketplace has been a very successful experience in this country. The American public can make millions of transactions in a highly complex marketplace with confidence. This can be attributed largely to the efforts of the participants of the National Conference on Weights and Measures during the past 74 years.

Today, decisions affecting retail equity are moving beyond the marketplace and presenting new measurement challenges. NBS has approached these challenges through a variety of mechanisms and found Standard Reference Materials (SRM's) to be particularly effective.

To discuss decisions affecting equity in this new arena, one must view the marketplace in a broader sense. All points of contact between parties where decisions are made which affect the end product must be considered. The traditional view of the retail market where buyer and seller meet to reach a decision and exchange goods is then just the final step in a long process.

What do we really mean by all of this? Step back from the sales arena for a moment to the point where products are being made, to the point where the quality of the product is being determined, where precise amounts of ingredients are blended, where parts are accurately welded together or assembled. At this point, quality control of the product is of importance. Equity here, as anywhere, means fairness; it is the assurance to both the producer and the consumer that the future performance



About 700 SRM's are currently used by industry to establish and maintain measurement quality control in the processing of raw materials as well as the processing and manufacturing of finished goods.

ance of the product will match expectations. This assurance can only be based on accurate and reliable measurements.

Quality Assurance for the Steel Industry

The role of measurement in quality assurance is readily illustrated in the high alloy specialty steel industry. Specialty steels require precise amounts of certain metals such as chromium and nickel to achieve their desired properties. Steels are produced in discrete batches. Toward the end of each batch process, a sample of the molten metal is dipped out and sent to a quality control laboratory for analysis. In this laboratory, measurements must be performed very rapidly while the bulk of the metal is held in a molten state. Adjustments to the composition of the steel can then be made to meet the desired specifications before the metal is allowed to cool and harden.

The key to equity in this example is the reliable determination of the chemical composition of the sample in the laboratory. In the steel industry, this determination is made via a direct comparison of the composition of the unknown steel sample with the composition of a standardized reference sample following an agreed upon test procedure. For specialty steels, it is clear that direct analysis of composition is required. But special alloys represent only a small component of the steel market and quality control is equally important for the large volume, low alloy steels used for auto bodies, girders and pipelines. NBS has worked on problems of quality control with the steel industry for over 75 years and has found that Standard Reference Materials are an effective way to transfer our measurement technology to the industry. The Bureau now offers over 100 different steel reference materials covering a wide variety of important compositions.

As indicated earlier, one must remember that these Standard Reference Materials by themselves do not make a complete measurement system. They must be used with a standardized measurement procedure which spells out how the comparison of the unknown sample with the reference sample



should be performed. In the case of steel, these procedures reflect industry consensus and are developed by voluntary standards organizations such as the American Society for Testing and Materials. Industry consensus is also important here for another reason since comparative tests like these are used by purchasers of steel for acceptance testing. Acceptance testing leads to a second decision point in the steel industry where equity issues are raised. Penalties are sometimes written directly into contracts for small deviations from the specified quality and acceptance tests are the agreed upon means of assessing these deviations.

Toxic Contaminants in Foods

In other segments of the economy, measurements have more subtle ways of affecting the quality of products. For example, in the food industry, questions have recently been raised about contamination of fruits and vegetables grown near sources of urban pollution. Leafy vegetables, such as lettuce and spinach, grown near industrial plants or highways are reported to acquire potentially harmful surface contaminations which are difficult to remove by washing. Also, toxic contaminants such as heavy metals are found in the soil and may eventually be absorbed into the plant tissue itself. The quantitative determination of the extent of this contamination requires accurate data on the trace element composition of fruits and vegetables grown at various



The Bureau has developed SRM's and definitive methods for most of the important components in blood, including glucose, urea, and sodium, that are used by physicians to diagnose and treat disease.

locations in both clean and polluted environments. The problem is further complicated by the fact that certain substances, such as chromium, are known to be toxic at one level but are essential nutrients at lower levels. Thus accurate analysis of the plant or food product is critical. In response to these measurement challenges, NBS has developed a series of biological reference materials. One material offered as part of this series consists of dried and pulverized spinach which has been carefully analyzed for trace elements. The spinach samples are used to calibrate analytical instruments that are used in turn for studying the effects of the environment on the food products already mentioned.

Accuracy in Clinical Chemistry

Personal services represent a very significant fraction of the American economy and once again sound measurement plays a key role. In the health care industry, for example, medical decisions are frequently based on the results of clinical laboratory tests. Nearly 4 billion individual measurements are made annually in conjunction with these tests in hospitals and clinical laboratories throughout the country. The estimated cost to the consumer is \$8 billion. The accuracy of such measurements is of paramount importance to both the physicians and their patients since the analytical results form the basis for an evaluation of the patients' health. NBS offers more than 30 different Standard Reference

Materials to clinical chemists to help calibrate their instruments and thus improve the accuracy of these critical measurements. These same Standard Reference Materials, along with companion reference methods, also provide the basis for regulation by the Food and Drug Administration (FDA), as well as for proficiency testing of clinical laboratories.

The importance of proper measurement can be brought into perspective by means of a specific example. There are approximately 2 million victims of epilepsy in the U.S. at the present time. In most cases, epilepsy can be fairly well controlled with drugs. However, in the past, the accuracy of laboratory tests for determining the proper drug dosage for each patient was extremely poor and many doctors chose to simply rely on the patient's reaction to the drug as their guide. In the fall of 1978, NBS issued a new anti-epilepsy drug SRM which consists of a set of 4 vials of freeze-dried human serum. Three of the vials contain 4 important anti-epilepsy drugs at different concentration levels: toxic, therapeutic, and sub-therapeutic. The 4th vial is a serum blank. With this set of reference materials, a clinical laboratory is able to analyze a sample of a patient's blood with assured accuracy and thus assist the physician in establishing the exact dose required for proper therapy. Thus, the health care received by the patient can be optimized with minimal side effects.

Environmental and Occupational Regulations

There is another decision point well beyond the marketplace where the question of equity is raised. That is the point where regulatory decisions are made. Many new laws have been enacted in the past decade that affect environmental regulation. By far the most significant Federal laws are the Clean Air Act of 1969, the Federal Water Pollution Control Act of 1972, and the Occupational Health and Safety Act of 1970. The economic impact of these laws is enormous. The Council on Environmental Quality estimates that the nation will spend \$486 billion in the period between 1975 and 1981 to reach the environmental objectives alone. An additional \$25 to \$30 billion in capital costs will be

NBS is working with voluntary standards-setting organizations to provide standards for materials recovered from waste in order to increase acceptance for them in the marketplace.



associated with occupational health and safety for the same period. The regulatory measurement system associated with these laws is also very large. It includes not only Federal agencies and U.S. industry, but State and local governments as well. Standard Reference Materials can play a key role here in helping to achieve equity between the regulators and those who are being regulated. More than 80 NBS SRM's are currently being used to assure the accuracy and compatibility of environmental measurements.

Pollution and Fuel Economy

In another area, automobile pollution monitoring and mileage testing, 36 NBS gas SRM's are required to place the measurements on a firm basis. In emission testing laboratories all over the country, exhaust gases are collected and analyzed to determine the amount of each pollutant gas emitted per vehicle mile. The results of these tests are tremendously important. First, they are used to determine whether the vehicle meets the pollution emission standards required by the Clean Air Act. But that is not the only application. They are also used in an EPA formula to calculate the fuel economy value—or the gas mileage—for a particular make of automobile. These are the fuel economy estimates posted on all new car windows. They are required

by law so that the consumer has an accurate basis for comparative shopping. There is a further fuel economy regulation included in the Energy Policy and Conservation Act of 1975. It requires that each car manufacturer achieve a certain weighted, average fuel economy for his total product line in a given model year. If the manufacturer's average is short of the standard, the law prescribes a penalty of \$5.00 for each 0.1 mile per gallon (0.04 km/L) his average falls below the standard times the total number of cars produced in that model year. For a company like Ford, that is a potential penalty of about \$15 million for each tenth of a mile per gallon. From this example alone, one can begin to appreciate the fact that accurate and reliable measurements are essential to equitable regulatory decisions. NBS SRM's are the primary calibration standards for these exhaust gas measurements.

Regulatory decisions are still being made and significant measurement problems remain. For example, urban dust is known to be a harmful pollutant but it has not been characterized well enough to establish a sound scientific basis for control. Over a two-year period NBS collected 23 kg (50 pounds) of dust from the air over St. Louis, Missouri. After careful blending to insure homogeneous samples, the composition of the material was analyzed and the levels of certain critical heavy metals in the dust such as lead, iron, uranium, cadmium,

chromium, copper, and zinc were established. The resulting urban dust SRM is now being used as a tool to develop new analytical techniques in anticipation of regulations on respirable dust. In fact, lead is already being regulated and the urban dust SRM is providing the measurement assurance for equitable compliance.

Resource Recovery

New measurement challenges exist even in areas much closer to the marketplace. Waste disposal for large urban centers is rapidly becoming a serious problem, a problem where measurement technology will play a significant role. The City of San Francisco is an excellent example. Sanitary landfill sites within close proximity to the city have been impossible to locate. The nearly 1.8 million kg (2000 tons) of solid waste generated each day must be loaded on long-haul vehicles and transported to a landfill located in the city of Mountainview, approximately 50 km (30 miles) south of San Francisco. The Mountainview site has limited capacity. The next suitable land fill site will require even longer hauls in the face of rapidly rising transportation costs.

Of more importance in the long term may be the fact that precious resources are being wasted with our present disposal techniques. Approximately 70 percent of municipal solid waste is usable as a fuel. In addition, other precious resources, such as ferrous metals and aluminum are present in the waste stream in substantial quantities. The technology for recovery of these materials is now available, but serious market barriers exist. Large-scale resource recovery facilities are exceedingly expensive. Thus, before investments in recovery facilities can be expected, markets for the recovered materials must be assured. In order to assure these markets, technical specifications must be developed to classify the recovered products as to quality, uniformity, and use. NBS is already heavily involved in developing reliable measurement techniques to characterize such things as heat and ash content of refuse-derived fuels. Again, Standard Reference Materials will undoubtedly play a key role in assuring equity in many aspects of this unique marketplace.

NBS Standard Reference Materials

Thus, equity appears in many places. Fairness must be achieved at many points of contact where decisions are made. Many things are needed to achieve equity but certainly an approach based on



NBS now issues over 900 Standard Reference Materials in 70 major categories to help increase and assure the accuracy of measurements made to improve efficiency in industry, monitor the environment, and improve health care.

measurements is a vital component. One measurement mechanism which NBS has found successful is built around Standard Reference Materials—materials produced in quantity, with one or more chemical or physical properties measured and certified by NBS. The 1979 sales of these materials is expected to reach a total volume of 38 000 units. These will be purchased by 10 000 different laboratories, 25 percent of which are in foreign countries. The Bureau's highest volume of sales in a single category has traditionally been in industrial quality control. The fastest growing categories in sales are in the clinical and environmental areas. In each of these categories, measurement plays a key role in the large arena beyond the marketplace.

Standard Reference Materials are but one of the measurement services that NBS will continue to offer to help develop accurate and reliable measurement capabilities to meet the challenges of the future. □

Mathematical models of energy and the economy are favored aids of government and industry planners but how "good" are the prophecies based on them?

Energy Forecasting: Improving on the Crystal Ball

by Michael Baum



A faint reflection of various acronyms and model names is visible on the surface of the crystal ball, including: MOGSM, WEM, LEAP, PILOT, STPPCDM, TESOM, LEAP, PILOT, STCRM, EOGRMS, FOSSILS, ETA-MACRO, EFS, BNL/DJA, PIES, TRENDLONG1995, RDFOR, TESOM, LEAP, PILOT, MOGSM, STPPCDM, BNL/DJA, and others.

PIES, MEMM, MOGSM, AHM, EOGRMS, TRENDLONG1995, RDFOR, STPPCDM, WEM, FOSSIL2, ETA-MACRO, TESOM, LEAP, PILOT, STCDM, MEFS, BNL/DJA . . .

Some people may recognize these immediately as computer programs by the acronymic insistence on capital letters, but they are more than that. These . . . entities are the crystal balls used by the modelers who are becoming the new prophets of our time.

These programs, the Project Independence Evaluation System, the Midterm Energy Market Model, and the others, are computer models of energy and economic systems for the United States. These programs are tools that help analyze what will happen to our fuel supplies—and fuel prices—next year, or 10 years from now, or 50 years from now.

More than that, the models analyze how those forecasts will be affected if certain factors, such as Federal regulations, are changed today. The results are used by policy makers in both government and industry in making crucial decisions about our nation's energy supply—the Department of Energy alone uses over 100 such models. But how valid are they?

This is a problem for specialists in a field called operations research, and among the handful of such groups studying the question is a team in the

Baum is a writer and public information specialist in the NBS Public Information Division.

COVER STORY

NBS Center for Applied Mathematics. "We're concerned with how you test the computer implementations of mathematical models used to aid decision making," says the project leader, Richard Jackson, "and we've had a long-term interest in large-scale models such as those the Department of Energy is using."

A model, in the operations research sense, is a set of mathematical equations which describes a real-life situation. It could be virtually anything—fire evacuation routes in a public building, the distribution of police patrol cars in a city, the organization of a large company, or the energy resources and allocations of a state, region, or nation.

Development of a model starts with the collection of data—such as the number of producing oil wells, rates of production, rates of discovery, refinery capacity, competing sources of energy—and a series of assumptions about how things work. The model combines these data and assumptions into a set of mathematical formulae which can be used to calculate some future state of the system.

For example, how much oil will be produced by a certain future year from an already known and producing field? A model to answer that question would take into consideration the amount of oil already produced by the field and the time it took to produce it, as well as geologists' estimates of the amount of known oil still in the ground. The model would also have to account for the so-called "inferred reserves" which are additional amounts of oil in the field that will be discovered by exploratory drilling and other techniques.

One model which estimates inferred reserves uses "Hubbert's Equation" (after M. K. Hubbert, formerly of the U.S. Geological Survey). This equation, derived by examining data about past discoveries, calculates the expected amount of inferred reserves as a function of the amount of oil produced in a given amount of time. Another model then uses these estimates of inferred reserves, together with estimates of "proven" (known) reserves, takes into account some assumptions about the price of oil and the cost of production in five years, and derives an estimate of the amount of oil that will be produced by the field five years from now. This estimate might even be reasonably accurate.

But other factors can also affect the answer. Will the market for oil disappear in the next five years? Suppose a change in Federal pollution regulations makes the high-sulfur-content oil in another field more profitable, what happens then? Will the



owners of this oil field invest the necessary money to find and open up the "inferred reserves"?

Because these models are usually very complex, they are coded into computer programs so that machines can handle the otherwise impractically large number of calculations. When the computer models become very intricate or deal in large volumes of data, as in the case of the examples above, they become "large-scale models." The task of validating such large-scale models is very difficult.

This is a damned difficult job.

*First one guy tells me what to do,
and he sounds right; then another
fellow tells me to do the exact op-
posite thing, and he sounds right.*

—Warren Gamaliel Harding

In a typical debate over energy policy and regulations, all sides can be expected to back up their positions with figures produced by computer models, and understandably, the models often differ. Which is correct, if any? What do they mean?

Often, there's an underlying political or social issue. Differences lie in an assumption or goal that you either accept or don't accept. But a more fundamental question is whether the model is valid. Does it really do what it is supposed to do?

The question is not easy to answer and the reason for that lies in the incredible complexity of some of the large-scale models, particularly in the energy field. They are simply so involved that it is difficult

to know exactly what is happening in the model unless you happen to be one of the persons who designed it. "With the advent of powerful computers and the ability to handle large amounts of data in a complex fashion," says Jackson, "it has become very difficult for another scientist to repeat or verify an experiment done using a large-scale model. This reproducibility is the foundation of the scientific method and without it, one loses credibility."

The NBS effort in this area is somewhat unique. At the request of the Department of Energy, the Operations Research Division is trying to develop a standard procedure, a set of guidelines, for evaluating large-scale energy models. If they succeed in coming up with a generally accepted set of procedures, it will be a first in the mathematical modeling field.

Members of the NBS Center for Applied Mathematics studying large-scale energy models include (right) Patsy Saunders and Lambert Joel and (below) Richard Jackson, Saunders, and Karla Hoffman.



Figure 1—These graphs represent the predictions of energy models typical of those used by the Department of Energy. The information used to make up the graphs comes from several models, including MOGMS, and shows how the natural gas supply in the U.S. may be expected to change in the future depending on certain changes in the supply and demand curves. Four different scenarios are presented for comparison: A—high demand, high supply; B—high demand, low supply; D—low demand, high supply; E—low demand, low supply. Scenario C (not shown) is for mid-range supply and demand.

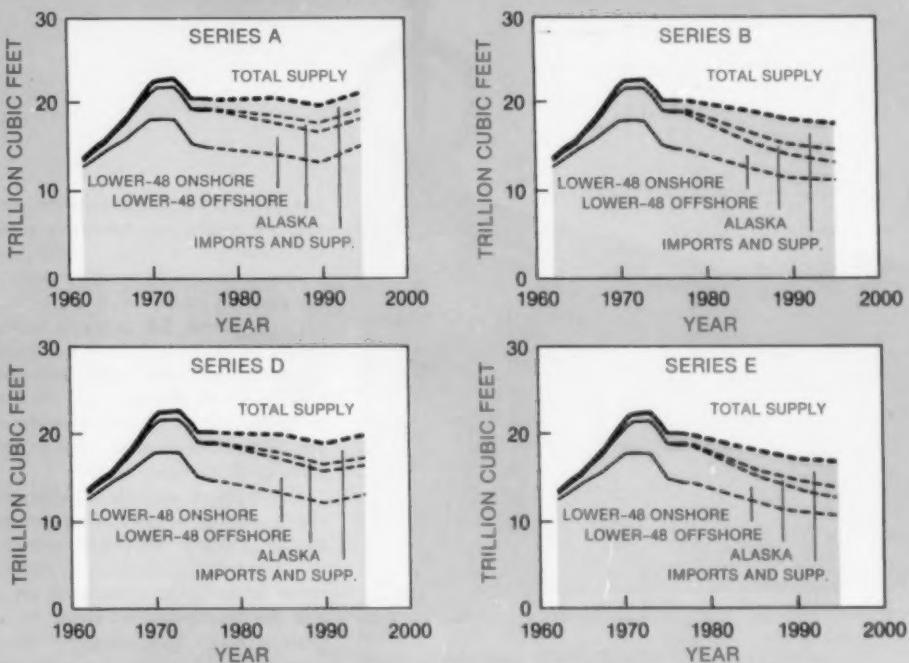
"A sort of transparency . . ."

"What we are promoting," explains mathematician Dr. Karla Hoffman, "is a sort of transparency for models—an understanding of the workings of models—so that policy makers can know on what their decisions are based. This field is new—modeling the energy environment got its great push forward in 1974—and some of the unanswered questions about models are not answered because the field is so new and research about the behavior of the process is in its infancy."

The approach the NBS team is taking is to develop an analysis of a representative energy model used by DOE and to record carefully each step of the process, false starts as well as successes, in the hopes of learning which steps are the most successful in bringing this transparency to large-scale models.

To understand the problem better, let's consider the model with which the NBS team is working. MOGMS, the Midterm Oil and Gas Supply Modeling System, is a major modeling system. It is used by the DOE's Energy Information Administration

U.S. NATURAL GAS SUPPLY BY SOURCE HISTORY AND PROJECTION SERIES, 1962-1995



(EIA) to develop projections of domestic oil and natural gas production for 15 years. The figures from this model are fed into two even more comprehensive models, the Midterm Energy Forecasting System (MEFS) and the Midterm Energy Market Model (MEMM). Estimates based on these systems and others become part of the EIA's Annual Report to Congress.

To those unfamiliar with large computer programs, it sometimes seems incredible that the users of these programs can't always be sure of what the program is doing, but let's look at the problem posed by something like MOGMS.

For one thing, the coding of a computer program, like any other creative activity, is intensely idiosyncratic. Every code bears the mark of the habits and prejudices of its writer. MOGMS has had several such creators.

The model was originally built in 1971 by the National Petroleum Council. In 1975 MOGMS was adopted by the then Federal Energy Administration (FEA) and modified to become part of the Project Independence Evaluation System (PIES). A year later, the program was changed again by FEA and a private consulting firm to include new inputs to the model. It was expanded yet a third time in 1977 by the consulting firm, and then reduced somewhat by DOE in 1978 when some unused or outdated portions of the model were eliminated. This is the point at which the NBS project received the model (it has changed a little since then) and

it is safe to say that there is no longer any person who completely understands every line of the computer code.

MOGMS is a midterm model. Such models are used to make predictions from about 5 years from now until the turn of the century. EIA uses three distinct types of predictive models, the short-term models that look 18 months to two years into the future, the midterm models, and the long-range models for the year 2000 and on. "They're looking at different things," explains Hoffman. "Short-term models are concerned primarily with demand behavior. What will be the immediate response in fuel consumption to changes in weather conditions, regulations or fluctuations in prices tomorrow? Things which require a long development period, like exploratory drilling or technological advances in synthetic fuels, won't have much effect on short term behavior. They may, however, significantly affect longer range predictions."

MOGMS is also basically an "engineering model," which means it makes its projections by actually trying to simulate the process of oil and gas development.

"Typically, models rely either on looking at what happened in the past and extrapolating to the future, or on trying to model, mathematically, the process that happens in the real world and predicting on the basis of that," according to Jackson.

"An 'engineering model' is a simulation of the process. The other kind, usually referred to as an



econometric or statistical model, uses past data and extrapolates a trend. There is an implied assumption in econometric models that anything that affected those past data will continue to do so in the future. Surprises, such as sudden price hikes or revolutions, throw off those models, while engineering models, on the other hand, can, if they are sufficiently detailed, take surprises into account.

"If you don't expect surprises, econometric models can be easier to use and more accurate, but the more complicated engineering models give you insight into the process. In making decisions about changes in regulations, you are considering imposing or removing a restriction on the process, so you don't want things to happen as they did in the past. In this case you use the engineering model. It's called the 'what if' process."

*It has long been an axiom of mine that
the little things are infinitely the
most important.* —Sherlock Holmes

There are, according to Jackson, two basic lines of study in validating a computer model: how valid was the original formulation of the model—does it make good assumptions about the process in the real world; and, how accurately does the computer program reflect the model?

Part of the problem, especially with a long-lived, many authored model such as MOGSMS, is in tracing the original source of an assumption or a number. "For example," says Jackson, "one of the assumptions made in this model is that the oil industry requires an 8 percent return on investment—above that they will invest, below that they won't. Well, that's an important number. Its rationale is

not given in the documentation, nor is it explained that the results are extremely sensitive to this assumption."

Now if the model were properly "transparent" to the decision makers who rely on it, that figure of 8 percent would be properly documented: there would be notes to inform the model user that the assumption had been made, and why it was thought to be justified. Beyond that, the assumption would be tested for its sensitivity in the model. Suppose you use 6 percent, or 10, how much difference does it make to the final results?

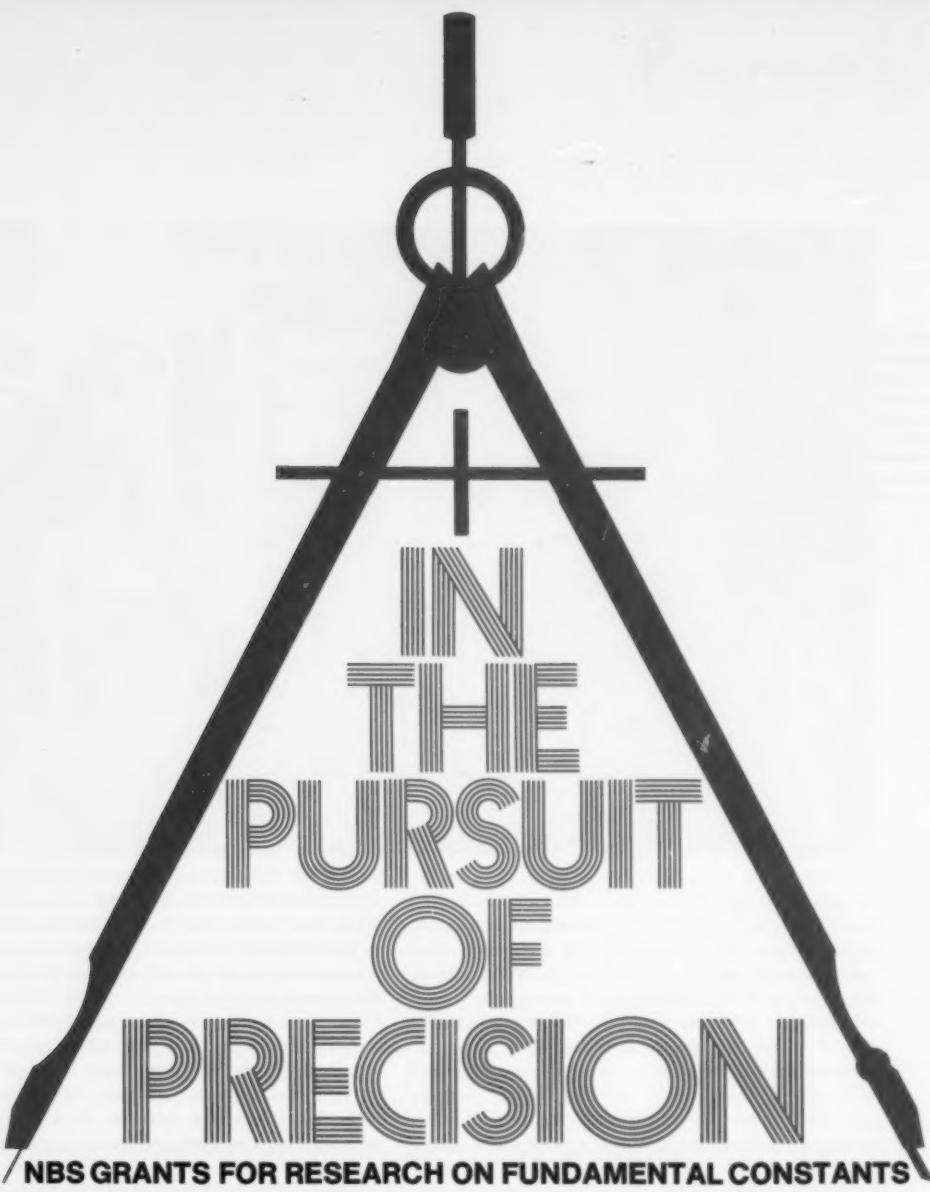
This type of analysis is what the NBS group is doing, and it's a painstaking and infinitely detailed sort of business. MOGSMS occasionally makes use of "Hubbert's Equation" mentioned above. But these factors were calculated on a national basis and the model applies them on a regional basis. Does it make a difference? "The purpose of the study," says Hoffman, "is not to determine that this model is either good or bad but rather to understand what the model is simulating, how well it achieves its purposes, and how it compares with others of its kind."

Finally, say the mathematicians, it is important for people using these models to understand what they can and cannot do.

For one thing, they say, the models are much better at looking at processes than at giving final figures. "There are very few modelers who believe the exact numbers that they get," explains Hoffman, "but they do believe the trends—whether the values tend to go up or down in a given situation."

"There are sometimes tremendous debates over the numbers that come out," Jackson agrees. "It says '14,' should it be 12 or 18? That isn't really the right question to ask. People think there is some magic to the numbers, but the real value of modeling is not the numbers that come out, but the fact that it provides a structure for debate." □

The NBS analysis of the Midterm Oil and Gas Supply Modeling System (MOGSMS) will be available in a few weeks. A good discussion of some of the topics mentioned in this article may be found in NBS Special Publication 534: *Utility and Use of Large Scale Mathematical Models*, the proceedings of a workshop held at NBS on April 28 and 29, 1977. SP 534 is available from the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402, for \$4.25. Request stock number 003-003-02060-5.



THE National Bureau of Standards has awarded two Precision Measurement Grants for research which will lead to improved values of several fundamental physical constants, including the gas constant, the Rydberg constant, and the electron-proton mass ratio.

The grants of \$25 000 each were awarded to William Sauder, Chairman of the Department of Physics of the Virginia Military Institute, for the development of a new type of ultrasonic interferometer; and to Carl Wieman of the Department of Physics of the University of Michigan, for the development of an extremely accurate system for atomic spectroscopy.

NBS Precision Measurement Grants have been awarded since 1970 to scientists in colleges and

universities engaged in research related to precision measurement and fundamental constants. The grants may be renewed for an additional two years, and while they often do not provide full funding for any one project, they are meant to encourage researchers to pursue those aspects of their work which involve precision measurements that might otherwise be ignored.

Sauder's work involves a redetermination of the gas constant, R, one of the fundamental constants of classical physics. R is best known to chemistry students for its use in the ideal gas law which states that the product of the pressure and volume of a gas is equal to the number of moles of the gas times its temperature times the constant R.

Professor William Sauder, Chairman of the Department of Physics at Virginia Military Institute, is shown with the Michelson-type ultrasonic interferometer he developed to make extremely accurate measurements of the speed of sound in gases. Sauder is flanked by students David Scherer, left, and Rick Fowler, right.



Traditionally, the value of R has been determined by physical chemistry experiments, but in recent years attempts have been made to measure the constant with greater accuracy through the use of ultrasonic interferometers— instruments which measure the speed of sound waves in the gas sample. (Such experiments rely on entirely different principles than the earlier chemistry experiments, and thus serve as a check on the accuracy of those measurements.)

Sauder's work is a refinement of the first interferometric measurement of the gas constant which was done in 1976 by Britain's National Physical Laboratory (NPL). That experiment, for a variety of technical reasons, proved to be a very difficult measurement. The first value differed significantly from the accepted value for R and occasioned three years of discussion and adjustment of the experimental data to account for errors inherent in the design of the equipment.

In remeasuring the gas constant by ultrasonic interferometry, Sauder will make use of a new instrument of his own invention which combines the idea of an ultrasonic interferometer with the design advantages of the double arm interferometer developed by A. A. Michelson in the early 1900's for his experiments on the nature of light waves.

The new instrument, according to Sauder, will significantly improve on the NPL experiment by avoiding two of the major sources of error in that measurement. (These were, first, the use of com-

paratively low frequencies which require fairly major adjustments to the data to satisfy the equations used to calculate R, and second, the presence of so-called "end effects" in the wave cavity of the interferometer which cause critical distortions in the sound field at either end of the instrument. Sauder's instrument is designed to operate at much higher frequencies, and the nature of a Michelson-type interferometer, which uses two wave cavities at right angles, tends to cancel out end effects.)

Sauder claims that when the ultrasonic Michelson interferometer is completed it will be able to make measurements of acoustic velocity with an accuracy of 10 parts per million or better, and will find many applications in thermometry and research on the properties of gases.

Wieman's project, in contrast, deals with some of the fundamental values of modern atomic physics, in particular the Rydberg constant and the electron-proton mass ratio.

Modern atomic theory holds that an electron in an atom can only have certain discrete energy levels, and that it may shift from one level to another as the atom absorbs or releases discrete amounts of energy. The Rydberg constant determines what those levels are, and therefore appears in most of the important equations of atomic physics. The ratio of the masses of the electron and proton is of similar significance.

Values for these constants are generally determined by analyzing simple spectra, such as that of



Dr. Carl Wieman of the University of Michigan is shown with part of the atomic spectroscopy equipment used in his experiment to measure the Rydberg constant and the electron-proton mass ratio.

the hydrogen atom, since certain lines in the spectrum correspond to the energy released by electrons shifting from one level to another. The technique is to "pump" energy into the atoms, usually with a laser that can be tuned across a range of frequencies, until the proper transition line (or "resonance") is found. Given an accurate value for that frequency, which corresponds to the energy involved in the transition, the value for the Rydberg constant can be calculated.

(Calculation of the electron-proton mass ratio is more complicated. It involves measuring how far a particular resonance line in the spectrum shifts between the spectra for hydrogen and for its heavier isotope, deuterium. The shift mirrors the effect on the electron of changing the mass of the nucleus.)

When experiments of this type are done to achieve very high levels of accuracy, a number of factors must be taken into account. Various processes in the atom, for example, tend to blur or broaden the spectral lines, making it difficult to determine the precise transition frequency. Additionally, a precise measurement of the frequency of the laser used as a reference is critical, and this is generally not a simple task.

Wieman's experiment takes the uncommon though not unheard of approach of measuring a three level resonance—that is, the electron absorbs energy in such a way that it goes from one level to a second, then to a third. In theory, the transition involved should have a narrow and well-

defined spectral line.

Wieman also avoids much of the difficulty in measuring the frequency of the laser by an arrangement that uses a combination of laser and radiofrequency radiation to pump the electrons to the proper energy level. Almost all the energy used in the transition (first level to second) is supplied by a dye laser beam, which intersects a beam of hydrogen atoms in a region that can be bathed with radiofrequency radiation. The laser can be very precisely fixed at one frequency (instead of being tuned across the spectrum), and the additional energy necessary to boost the electrons to the proper level (second to third) is supplied by tuning the radiofrequency source. This allows Wieman to make the final critical frequency measurement in the radiofrequency range—a much simpler task than measuring a frequency in the visible spectrum.

Wieman hopes to be able to determine the transition frequency to about three parts in 100 billion (10^{11}) and the corresponding hydrogen-deuterium isotope shift to about four parts in 100 million (10^8). If so, the resulting calculations would make the Rydberg constant the most precisely measured fundamental constant to date, and the values of several other related constants would be improved.

Those interested in the Precision Measurement Grant program can obtain further information from Dr. Barry N. Taylor, B258 Metrology Building, National Bureau of Standards, Washington, D.C. 20234. M.B.

ON LINE WITH INDUSTRY

NBS MEASUREMENT SEMINARS

NBS will conduct a series of Measurement Seminars during 1980 to furnish advice and assistance to the growing number of laboratories involved in making precise, accurate measurements for research, production control, or field evaluation.

Tailored to the working professional, these seminars provide practical experience and training in the problems of modern metrology and calibration. Emphasis is placed on tracing measurements to NBS standards at the appropriate level of accuracy for each application.

Measurements in fields such as time and frequency, thermometry, and physical dimensions are traditional subjects of the Measurements Seminars which began in 1963, and to these have been added in recent years such fields as electromagnetic interference and ionizing radiation measurements. The current 1980 Measurement Seminar Series includes 11 seminars on 8 topics.* A brief description of each is given below. Further information on the 1980 series can be obtained from Joanne Marshall, NBS Office of Measurement Services, Physics Building, Rm. B362, National Bureau of Standards, Washington, D.C. 20234, telephone: 301/921-2805.

Two seminars on the *Calibration and Use of Piston Gages* will be held in the Spring and Fall of 1980. Each 2-day seminar examines the theory of piston gages, elastic distortion, design and types of piston gages, various calibration procedures, error analysis, computer programs, a demonstration of cross-float calibration, hydrostatic weighing, and transducer calibration. Registration is handled by Bernard Welch, 301/921-2121.

The *Time and Frequency User's Seminar* will also be held in both Spring and Fall of 1980 and will cover topics including: the choosing of a calibration source; the organization of time and frequency in the U.S.; publications available from NBS and

the U.S. Naval Observatory; care and use of frequency sources; use of the Loran-C navigation system for frequency calibration; use of station WWVB for frequency calibrations; an introduction to TV and satellite calibration methods; and the time and frequency measurement services available from NBS. Registration is through George Kamas, 303/499-1000, ext. 3378.

Each of the two *Precision Thermometry Seminars*, which begin March 10 and September 8, is actually four courses in one. Over the course of five successive days, lectures, demonstrations, and laboratory instruction will be provided on platinum resistance thermometry (2 days), liquid-in-glass thermometry, thermocouple thermometry, and thermistor thermometry. Registration is through Nancy E. McBryde or James F. Schooley, 301/921-3315.

A 4-day seminar on *Micro-measurements on Integrated-Circuit Silicon Wafers*, presented from July 15-18, will be concerned with making accurate and precise measurements of IC linewidths. Topics will include the theory of optical microscopes (including operating conditions necessary for accurate measurement), data analysis, linewidth calibration, measurement artifacts, and the transfer of measurement standards from NBS to the IC industry. The primary emphasis is on measurements in the 0.5 to 10 micrometer range with a microscope operating in bright-field reflected light. Registration is through John M. Jerke or Elaine C. Cohen, 301/921-3786 or 3621.

A seminar on *Electrical Measurements at High Voltage Levels* will be held from April 1 to 3. Dealing with dc, 60 Hz, and impulse measurements, the seminar will cover such areas as the generation of test voltages and the influence of generator parameters on the accuracy of the measurements; the important characteristics of dc and impulse voltage dividers, transformers and capacitance-coupled voltage transformers; bridge circuits, transformer test sets, oscilloscopes, peak-reading voltmeters and digitizing data acquisition systems; and guarding, grounding and

shielding procedures. Registration is through F. Ralph Kotter, 301/921-3121.

Metrology of Modern Electronic Instrumentation is the title of a seminar held from May 13 to 15 on precision waveform sources, accurate data acquisition, and measurement processing applications. Topics to be covered include special purpose signal generators, phase angle standards, data acquisition and conversion, digital signal processing, interface standards, automatic calibration systems, and Automated Test Equipment (ATE) applications. Registration is through Barry A. Bell, 301/921-2727.

A seminar on *Traceability for Ionizing Radiation Measurements* will be held on May 8 and 9. Discussion will center around how measurements of ionizing radiation may be traced to the national standards maintained by NBS. Current NBS services and concepts for improved criteria and mechanisms will be covered as well as tracing measurements through various institutions that function as secondary standards laboratories. General concepts of traceability will be presented followed by specific applications in medical, environmental, and occupational areas of concern. Registration is through H. T. Heaton, II, 301/921-2551.

Finally, on July 22 to 24, NBS will present an *EMI Metrology Seminar* on the instrumentation and measurement techniques for monitoring electromagnetic interference (EMI). Subjects will include instrumentation for characterizing and simulating the EM environment and techniques for measuring emissions and susceptibility of electronic equipment. Registration is through M. Gerald Arthur, 303/499-1000, ext. 3603.

Enrollment in these seminars is generally limited, since the emphasis on "hands on" laboratory training restricts the number of participants that can be accommodated at any one time. Individuals from measurement and standards laboratories who must regularly make precise measurements in their work and who have appropriate prerequisites in education and experience are particularly encouraged to attend.

M.B.

*A twelfth seminar, on Measurement Assurance for Gage Blocks, has already been held.

STANDARD STATUS

GAS SRM'S FOR EMISSIONS TESTING OF HEAVY DUTY VEHICLES

In a major project to help standardize emissions testing of heavy duty motor vehicles, NBS has completed certification of 13 new gaseous Standard Reference Materials (SRM's). The goal of the two-year program, which is cosponsored by the Motor Vehicle Manufacturers Association (MVMA), is to conduct the necessary research, and to develop and produce a total of 26 new gaseous SRM's by July 1980.

The SRM's are gas mixtures of nitrogen with such gases as nitric oxide, carbon dioxide, propane or carbon monoxide in concentrations suitable for analysis of heavy duty motor vehicle emissions.

The need for these SRM's stems from the revised Clean Air Act passed by Congress in 1977. The goal of this law is to reduce the amount of carbon monoxide, nitrogen oxides and hydrocarbons contained in motor vehicle exhaust to 90 percent of their "pre-control" levels by 1981. The EPA published regulations in June 1977 requiring manufacturers of heavy duty vehicles (those with gross vehicle weight over 8,500 pounds [3856 kg]) to calibrate their emissions testing instruments with gases traceable to NBS gas standards.

The cooperative program with the MVMA, which provides for two full-time research associates from the specialty gas industry, was established to enable NBS to produce the new SRM's needed for manufacturers to comply with the regulations within the required time.

"Normally," says research associate Bill Thorn, "it takes years to put this many new SRM's on the shelf." Under the NBS/MVMA program, the production of gaseous SRM's has been accelerated with the extra personnel provided by the program.

Without the appropriate NBS SRM's to serve as "benchmarks," gas standards for emissions testing are obtained from a

variety of sources, making it difficult to assure compatibility among measurements made by the various vehicle manufacturers and the EPA. The availability of SRM's of the appropriate composition and gas concentrations assures that all measurements will be made against a common base. Concentration values in parts per million or percent by amount of substance in moles assigned to these SRM's are stated with an estimated uncertainty of not more than ± 1 percent of the value at the 95 percent confidence level.

The new SRM's produced by the program will either extend the range of, or provide standards with concentrations intermediate to, existing SRM's currently used in the analysis of automobile emissions. However, the majority of the new SRM's are of concentrations much higher than those used for automobile emissions testing.

NBS standard reference gas mixtures are prepared in lots of 50 by gas manufacturers according to specifications developed by NBS. Each sample is individually analyzed at NBS by carefully intercomparing the purchased cylinders with NBS primary laboratory standards.

The gases are supplied in aluminum cylinders, conforming to Department of Transportation specifications, with a delivered volume of gas between 700 and 870 liters at standard temperature and pressure.

A certificate supplied with each cylinder states a concentration value which is considered valid for at least two years from the date of purchase.

For further information, contact the Office of Standard Reference Materials, B311 Chemistry Building, National Bureau of Standards, Washington, D.C. 20234.

Gas SRM's to be produced under the NBS/MVMA program.^t

2627 NO in Nitrogen, 5 ppm	2641 CO in Nitrogen, 4 percent*
2628 NO in Nitrogen, 10 ppm	2642 CO in Nitrogen, 8 percent*
2629 NO in Nitrogen, 20 ppm	2643 Propane in Nitrogen, 100 ppm
2630 NO in Nitrogen, 1 500 ppm*	2644 Propane in Nitrogen, 250 ppm
2631 NO in Nitrogen, 3 000 ppm*	2645 Propane in Nitrogen, 500 ppm
2632 CO ₂ in Nitrogen, 300 ppm*	2646 Propane in Nitrogen, 1 000 ppm
2633 CO ₂ in Nitrogen, 400 ppm*	2647 Propane in Nitrogen, 2 500 ppm
2634 CO ₂ in Nitrogen, 800 ppm*	2648 Propane in Nitrogen, 5 000 ppm
2635 CO in Nitrogen, 25 ppm*	2649 Propane in Nitrogen, 1 percent
2636 CO in Nitrogen, 250 ppm*	2650 Propane in Nitrogen, 2 percent
2637 CO in Nitrogen, 2 500 ppm*	2651 Propane, 100 ppm, 5 percent O ₂ in Nitrogen
2638 CO in Nitrogen, 5 000 ppm*	2652 Propane, 100 ppm, 10 percent O ₂ in Nitrogen
2639 CO in Nitrogen, 1 percent*	* SRM's with complete certification at the time of publications.
2640 CO in Nitrogen, 2 percent*	

^t Concentrations are by amount of substance in moles.

* SRM's are well characterized materials or measuring devices which have one or more physical or chemical properties certified by NBS. SRM's are widely used for calibrating or testing all kinds of measurements.

EDDY CURRENT IMAGING SYSTEM

Scientists in the NBS Center for Absolute Physical Quantities have designed a prototype probe as part of an eddy current flaw detection system that could prove useful in nondestructive evaluations of metal products. Preliminary experiments indicate that the probe should provide information about the type and shape of surface flaws as well as limited data on sub-surface flaws.

Bruce F. Fields, Electrical Measurements and Standards Division, B258 Metrology Building, 301/921-3806.

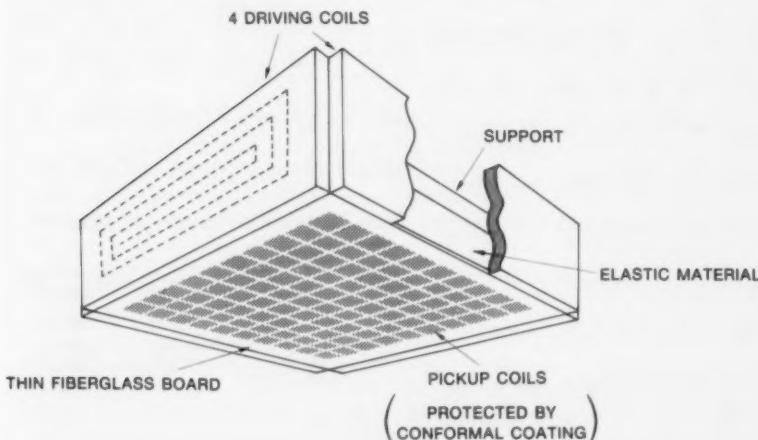
We initiated a project to develop an eddy current flaw detection system with a meaningful display and to demonstrate whether or not such a system could be used to determine the type and shape of flaws. This work started with a literature search for papers concerning defect detection or characterization using eddy current techniques. A promising approach for a sensor was reported by McMaster (Met. Eng. Quart. pp. 32-48, May 1966) using a Hall effect detector. We built a similar sensor and performed several experiments. As a result of these experiments and later discussions with Mc-

Master, we learned that pickup of extraneous signals by the leads to the sensor introduced significant problems. Adequate shielding of the leads proved difficult and appeared to be impractical for a large array of sensors, thus we decided the sensor design could be better met by a differential coil arrangement.

A probe assembly of our own design, consisting of an array of small pickup coils (about 50 coils) with 4 large driving coils arranged in a square around the array of pickup coils, has been proposed as a possible flaw detector. The present implementation of this idea is shown in Figure 1, a drawing of a prototype probe assembly; this assembly is placed on the flat surface to be analyzed. Driving coils on opposite sides of the array will be excited simultaneously but with current signals 180 degrees out of phase with each other. By varying the relative signal strength of the two coils, we should be able to detect conductivity discontinuities with high spatial resolution. Information about the shape of the discontinuity can be obtained by separately energizing the orthogonal pair of driving coils.

This idea, as yet, is untested, however; preliminary experiments indicate that this is a feasible concept. Potential advantages of this concept are:

Figure 1—Prototype probe assembly for the eddy current imaging system.



- 1) The assembly allows high spatial resolution of discontinuities with a relatively small number of pickup coils.
- 2) A reasonably large area (approximately 80 cm² in the prototype) can be analyzed without mechanical scanning.
- 3) The system will provide limited information about the shape of the discontinuity, i.e., it will distinguish between cracks and pits.
- 4) The test is most sensitive to surface discontinuities; however, limited information about subsurface discontinuities and the depth of the discontinuity may be available.
- 5) The prototype is designed for flat surfaces, but a modification of the probe will also allow testing of slightly curved surfaces.

A desktop computer will perform experiment control, data logging, and data reduction for the system. The computer has been interfaced successfully to a frequency synthesizer (for energizing the driving coils) and a general purpose interface crate of our own design. The interface crate allows us to interface easily a variety of instruments to the computer. We have the ability at present to perform data logging of 8 analog channels (with 0.025% accuracy) and to control a mechanical scanner. Several computer programs have been written to perform a one-dimensional scan of an aluminum plate, digitize the signals from the pickup coils, and graphically display the results. A lock-in analyzer is used to amplify and phase detect the in-phase and quadrature components of the pickup coil signals. These mechanical scanning experiments were used as a convenient method for examining eddy current fields. Using the information gathered in these experiments, we were able to produce an improved design for the pickup coils.

ECONOMICAL AND ACCURATE METHOD FOR CALCULATION OF ATOMIC PROPERTIES

Many-body perturbation theory (MBPT) is a systematic approach to the accurate

calculation of atomic properties such as energy levels, transition probabilities, polarizabilities, and photoionization cross sections. MBPT attempts to solve a complicated problem in atomic theory by reducing it to the combination of a simpler problem plus a well-defined series of successively smaller correction terms (perturbations). Traditional methods for implementing MBPT have seldom allowed consideration of more than two or three such correction terms, due mainly to the large amount of computer time required for their evaluation. Recent work at NBS has resulted in a new numerical technique—the contracted orbital formulation of many-body perturbation theory (COMBPT)—which reduces the cost involved in calculating higher-order corrections by as much as 90-95 percent, while yielding accuracies equal to or exceeding those obtained with standard methods. This development should bring many hitherto unapproachable problems in atomic theory within reach of the powerful many-body formalism.

Stephen M. Younger, Atomic and Plasma Radiation Division, A267 Physics Building, 301/921-2071.

The Bruckner-Goldstone formulation of many-body diagrammatic perturbation theory is a powerful technique for the accurate calculation of a variety of microscopic quantities. In applying this method to atoms involving two or more electrons, one first defines an approximate zeroth order Hamiltonian for the system, with its associated complete set of eigenfunctions. Eigenfunctions corresponding to physically occupied orbitals are termed "hole" states; the remainder of the complete set constitutes the "virtual" (i.e., not physically occupied) set. This basis set is then used to evaluate the matrix elements appearing in the perturbation expansion for the exact energy or wavefunction.

While such procedures are reasonably straightforward to apply, one finds in practice that extremely large basis sets are required in order to obtain conver-

gence of the perturbation expansion, usually in the range of five to ten bound states and 15 to 30 continuum states. When evaluating the particle-particle interaction appearing in higher order (>1) perturbation terms, such a set requires the calculation of several hundred thousand matrix elements per diagram, many of which involve integrations over products of continuum functions.

The key to cutting this problem down to size is to generate a small but reasonably complete set of basis functions which adequately describes correlation within the atom. We found that one way of doing this is to restrict the radial range of the virtual orbitals by the construction of a potential barrier about the atom. Therefore, we have defined a "contracted" zeroth order Hamiltonian such that the virtual states see the zeroth order potential modified by an exponential barrier beginning at some radius R_w .

The barrier is placed sufficiently far from the nucleus that the physically-occupied orbitals are left unaffected. The virtual set, however, consists entirely of discrete states of finite radial extent—an attribute which greatly simplifies their numerical calculation and use in the perturbation expansion. Such a formulation of MBPT produces a complete set only in the radial region required to describe correlation effects within the atom, and eliminates the necessity of computing large numbers of long range virtual orbitals which add only to the complexity and not to the accuracy of bound state calculations.

We have applied the "contracted orbital" formulation of many-body perturbation theory (COMBPT) to the calculation of correlation energies and transition probabilities in a number of simple atoms and ions, including H⁺, He I, Be I, N IV, Ne VII, and Ne I. The results of some of these calculations are given in table 1.

Transition probabilities for ions in the palladium isoelectronic sequence have also been evaluated. In all cases, three to

eight virtual orbitals—rather than the 20-30 needed with the traditional techniques—were found adequate to ensure convergence with respect to the basis set size. A simple but accurate extrapolation procedure for including contributions from higher virtual orbitals has been devised. With such small basis sets, it is possible to achieve a 95 percent reduction in computation time compared to the continuum basis formulation, with equal or greater accuracy.

The small basis sets occurring in COMBPT allow one to compute routinely higher order correlation diagrams which would be practically unapproachable by traditional atomic MBPT. The H⁺ correlation energy calculation was particularly interesting in that the COMBPT method eliminated a divergence—which occurs in the continuum basis techniques—in the summation of diagrams involving repeated hole-hole interaction. Using COMBPT, we found that the perturbation series for the 1s² correlation energy did not begin to converge until the fourth order, with oscillatory convergence in higher, even-numbered orders. This was one of the first calculations of such higher order correlation diagrams for atoms.

Although the contracted orbital method was developed primarily for application to bound state problems, the close resemblance of the virtuals to the inner loops of continuum functions suggests their use in a form of R-matrix theory of scattering processes. Such applications are currently being investigated.

Table 1
Comparison of correlation energies
(values given in atomic units*).

Atom	COMBPT	Best Previous Calculation
He	.04124	.04204
Be (2s-2s)	.04498	.0455
N IV (2s-2s)	.0832	.0855**
Ne VIII (2s-2s)	.1226	.1239**

* 1 atomic unit = 4.36×10^{-19} joules

** Estimated

RESOLUTION OF PHOTON-RECOIL COMPONENTS OF VISIBLE SPECTRAL LINE

Researchers at the National Bureau of Standards Laboratories in Boulder, CO, have taken a substantial step towards producing a very stable frequency or wavelength standard in the visible region of the spectrum. They have succeeded in resolving, for the first time, the photon-recoil components of a visible spectral line. Using saturated absorption spectroscopy on the 657.3-nm calcium line (the narrowest line ever resolved in the visible spectrum), this work shows the calcium beam to be potentially much better than the best present visible wavelength standard, the iodine-stabilized He-Ne laser.

Richard L. Barger, Time and Frequency Division, Room 1-3530, NBS, Boulder, CO 80303, 303/499-1000, ext. 3404.

Saturated absorption spectroscopy has been used extensively to eliminate the Doppler broadening due to the thermal

motion of atoms. Using saturated absorption techniques with a beam of calcium atoms, they have achieved sufficient spectral resolution to observe the minuscule broadening caused by the photon-recoil effect.

When an atom absorbs a photon, the atom recoils in the same direction as that of the incoming photon. Later, when another photon stimulates the atom to emit a photon, the atom recoils in the opposite direction to the first movement. These tiny recoil movements cause Doppler shifts that have never before been observed at visible frequencies.

These recoils in opposite directions cause the single narrow absorption line to be observed as two components, shifted slightly above and below the natural frequency. The components are separated by 23 kHz (the frequency of the 657.3-nm line is 456×10^{12} Hz), and their resolution permits measurement of the center of the line to within 300 Hz or better.

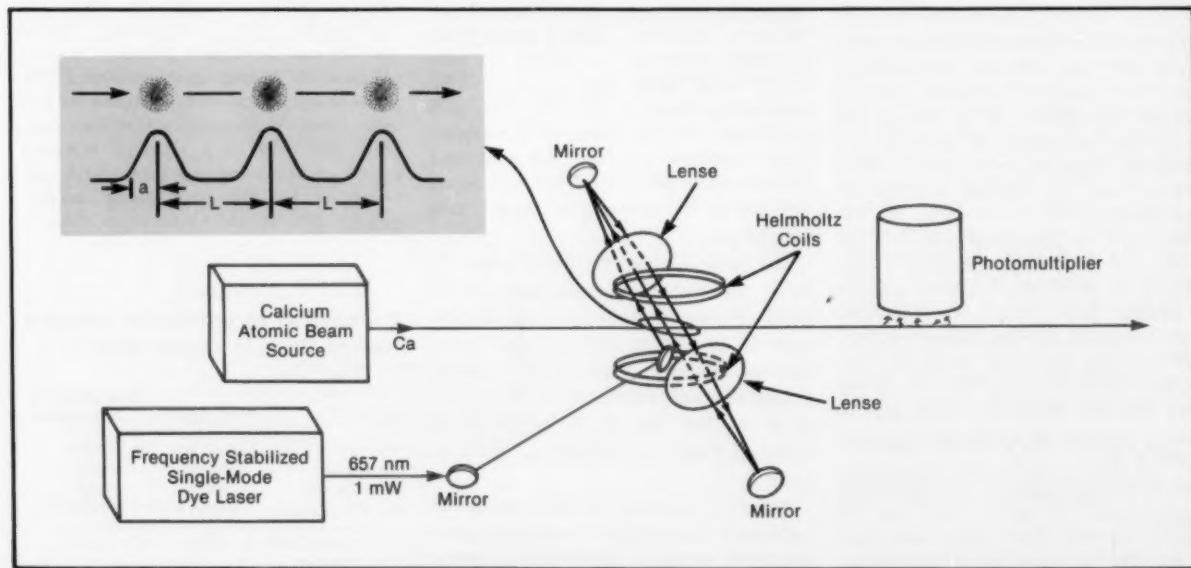
The apparatus which was used consists of a series of lenses and mirrors in a "cat's eye" arrangement (see figure 1) which causes the laser beam to pass through the calcium beam on three precisely parallel

paths. Each path is traversed in both directions by the photons being absorbed and emitted. The resulting three zones of interaction between calcium atoms and photons produce optical Ramsey fringes which give simultaneously high resolution and high signal-to-noise ratio.

Further refinements, such as the measurement of the second-order Doppler shift, could result in reducing the systematic errors to less than one part in 10^{14} , making the calcium beam an extremely accurate frequency/wavelength standard. The natural linewidth of the transition ($^1S_0 - ^3P_1$) is only 410 Hz, one of the narrowest known in the visible region, and therefore, a logical candidate for investigation as a standard.

In addition to the usual applications of such standards, the calcium beam might be useful in improving certain tests of relativity or fundamental constants.

Figure 1—The "cat's eye" arrangement of lenses and mirrors causes the laser beam to follow precisely parallel paths through the calcium beam. Each path is traversed in both directions by the photons. Using three interaction zones gives high resolution and good signal-to-noise ratio. Inset: Gaussian laser beam profiles at the three interaction zones.



CONFERENCES

For general information on NBS conferences, contact JoAnn Lorden, NBS Public Information Division, Washington, D.C. 20234, 301/921-2721.

WORKSHOP ON COMPUTER INTERFACE STANDARDS

The National Bureau of Standards technical workshop on Federal input/output (I/O) computer interface standards, originally scheduled for November 1 and 2, 1979, at NBS headquarters in Gaithersburg, Maryland, has been rescheduled for March 3 and 4, 1980, to permit wider participation. Existing and future Federal computer I/O interface standards will be discussed including:

- Performance enhancement of Federal Information Processing Standard (FIPS) 60 (*I/O Channel Interface Standard*), with emphasis on implementation techniques supporting data transfer rates in the range of 5 to 10 megabytes per second.

- Electrical, logical, and other specific limitations of FIPS 60 relative to data transfer rate and other performance-related constraints.

- Suggestions for new operational specifications standards to accompany FIPS 60, similar to FIPS 62 (*Operational Specifications for Magnetic Tape Subsystems*) and FIPS 63 (*Operational Specifications for Rotating Mass Storage Subsystems*). Technical specifications for new classes of magnetic disk storage systems, expected to be in widespread use over the next several years, would be of particular interest.

- Means of specifying those channel level device class specific interface characteristics that are necessary to assure interchange of peripherals, while allowing peripheral subsystems to have open-ended storage capacity and other enhanced capabilities, such as buffer storage.

Inquiries concerning the workshop should be addressed to William Burr, B212 Technology Building, NBS, Washington, D.C. 20234, 301/921-3723.

COMPUTER NETWORK PROTOCOLS SYMPOSIUM

Papers are now being solicited for the "Trends and Applications 1980: Computer Network Protocols Symposium" to be held at the National Bureau of Standards

in Gaithersburg, Maryland, on May 29, 1980.

The event is cosponsored by the NBS Institute for Computer Sciences and Technology, the Washington, D.C., chapter of the Institute of Electrical and Electronics Engineers (IEEE) Computer Society, and the IEEE Washington Section.

In particular, the program committee is interested in papers of a tutorial nature and those that present new research in areas including:

- architectural models
- individual protocol models
- high-level protocols
- transport/backbone network protocols
- verification
- standardization
- performance evaluation

For further information contact Helen M. Wood, Conference Chairperson, NBS, A209 Administration Building, 301/921-2834 or Fran Nielsen, Conference Vice-Chairperson, NBS, B212 Technology Building, 301/921-2601.

CONFERENCE CALENDAR

March 3-4

WORKSHOP ON COMPUTER INTERFACE STANDARDS, NBS, Gaithersburg, MD; sponsored by NBS; contact: W. E. Burr, B212 Technology Building, 301/921-3723.

*April 16-18

CONFERENCE ON FIRE ENGINEERING, NBS, Gaithersburg, MD; sponsored by NBS; contact: Irwin Benjamin, B250 Polymers Building, 301/921-3255.

May 1-2

IMPLANT RETRIEVAL: MATERIAL AND BIOLOGICAL ANALYSIS, NBS, Gaithersburg, MD; sponsored by NBS, DOC, FDA, DHEW, VA, and ASTM; contact: A. W. Ruff, B118 Materials Building, 301/921-2966.

May 5-7

TOPICAL CONFERENCE ON BASIC OPTICAL PROPERTIES OF MATERIALS, NBS, Gaithersburg, MD; sponsored by NBS in cooperation with OSA; contact: Albert Feldman, A251 Materials Building, 301/921-2840.

May 13-15

MEDILOG 80, NBS, Gaithersburg, MD; sponsored by NBS and DOD; contact: Charles Hulick, A740 Administration Building, 301/921-3465.

*May 29

IEEE COMPUTER CONFERENCE, NBS, Gaithersburg, MD; sponsored by NBS and IEEE; contact: Frances Nielsen, B212 Technology Building, 301/921-2601.

June 2-6

6TH INTERNATIONAL CONFERENCE ON VACUUM ULTRAVIOLET RADIATION PHYSICS, UNIVERSITY OF VIRGINIA, CHARLOTTESVILLE, VA; sponsored by NBS, NRL, University of Virginia, NSF, DOE, IUPAP; contact: Robert Madden, A251 Physics Building, 301/921-2031.

June 2-4

FIFTH INTERNATIONAL SYMPOSIUM ON ULTRASONIC IMAGING AND TISSUE CHARACTERIZATION, NBS, Gaithersburg, MD; contact: Melvin Linzer, A366 Materials Building, 301/921-2611.

June 4-6

SECOND INTERNATIONAL SYMPOSIUM ON ULTRASONIC MATERIALS CHARACTERIZATION, NBS, Gaithersburg, MD; sponsored by NBS and ASNT; contact: Harold Berger, B312 Physics Building, 301/921-3331.

June 19

19TH ANNUAL TECHNICAL SYMPOSIUM: PATHWAYS TO SYSTEM INTEGRITY, NBS, Gaithersburg, MD; sponsored by NBS and ACM; contact: Carol Wilson, A252 Technology Building, 301/921-3861.

*New Listings

PUBLICATIONS

BUILDING TECHNOLOGY PUBLICATIONS CATALOG

Debelius, J. R., *Building Technology Publications—Supplement 3: 1978*, Nat. Bur. Stand. (U.S.), Spec. Publ. 457-3, 106 pages (July 1979) Stock No. 003-003-02096-6, \$4.00.*

From solar heating and cooling test methods to fire resistance of concrete and life-cycle costing analysis, a wide variety of topics are treated in the more than 200 writings described and indexed in the 1978 publications catalog from the Center for Building Technology at the National Bureau of Standards.

Complete with capsule descriptions of the papers, articles, and booklets as well as author and key-word indexes, the catalog groups the entries into categories including: NBS Building Science Series, Technical Notes, Special Publications, Handbooks, Interagency Reports, Government Contract Reports, and papers published in non-NBS media.

* Publications cited from this point on may be purchased at the listed price from the U.S. Government Printing Office, Washington, D.C. 20402 (foreign: add 25%). Microfiche copies are available from the National Technical Information Service, Springfield, VA 22161. For more complete periodic listings of all scientific papers and articles produced by NBS staff, write: Editor, Publications Newsletter, Administration Building, National Bureau of Standards, Washington, D.C. 20234.

STABILITY OF (THIN FILM) SOLAR CELLS AND MATERIALS

Sawyer, D. E., and Schafft, H. A., *NBS/DOE Workshop, Stability of (Thin Film) Solar Cells and Materials*, Nat. Bur. Stand. (U.S.), Spec. Publ. 400-58, 181 pages (Aug. 1979) Stock No. 003-003-02100-8, \$5.00.

This is a collection of 18 papers and the reports of three discussion groups which were presented at the NBS/Department of Energy Workshop on the Stability of (Thin Film) Solar Cells and Materials, in May 1978.

The workshop dealt with the problem of achieving and measuring the long-term stability of solar cells that use thin film materials and semiconductor device technologies. In general, the workshop identified the necessary work to be done in this field and divided it into two areas: the development of an improved understanding of cell operation and the component structures in these cells, and the development of an improved measurements base.

The discussions covered solar cell materials of three different groupings: (1) Cu₂[CdZn]S, Cu-ternaries/CdS, InP/CdS, and amorphous Si; (2) polycrystalline, metal-insulator semiconductor (MIS), and conducting-oxide Si; and (3) polycrystalline and antireflection-coated metal-oxide-semiconductor (AMOS) GaAs.

SLIDE PROGRAMS FOR ARCHITECTS ON NOISE, WINDOWS

Two audiovisual programs resulting from research conducted by the National Bureau of Standards' Center for Building Technology are now available for purchase or free loan. The programs, "Noise Control for Designers" and "Window Design Strategies to Conserve Energy," are geared toward the practicing architect and the architectural student.

"Noise Control for Designers" deals with the problem of noise in the home and office. It recommends ways for de-

signers and contractors to reduce the noise level through installation of quieter equipment, such as appliances and plumbing ducts, and use of noise absorbing materials, such as acoustical ceiling tile and wall installation. The show is available from the National Audio Visual Center, GSA, Reference Section, Washington, D.C. 20409, for \$48.00 (order #A0078).

"Window Design Strategies to Conserve Energy," a three-part program, delineates six strategies to make windows more energy efficient. Part one outlines window exterior strategies, part two, frames and glazing, and part three, interior strategies. Each strategy is designed to maximize at least one of the attributes of windows: passive solar heating, daylighting, shading, insulation, air tightness, and ventilation.

The set of three presentations, approximately 25 minutes each, costs \$65.00 (order #A00781). The programs are also available for free loan from Modern Talking Picture Service, 5000 Park Street North, St. Petersburg, FL 33709. Borrower pays return postage and insurance only.

COMPUTER PROGRAM DOCUMENTING PRACTICES, CRITERIA

Guidelines for Documentation of Computer Programs and Automated Data Systems for the Initiation Phase, Nat. Bur. Stand. (U.S.), Fed. Info. Process. Stand. Publ. (FIPS PUB) 64, 54 pages (1979). Available from National Technical Information Services, for \$5.25 (paper copies) or \$3.00 (microfiche copies).

Suggested practices for documenting computer programs, beginning with the early phases of software planning and evaluation, are detailed in a new guide issued by the National Bureau of Standards.

Developed by the Bureau's Institute for Computer Sciences and Technology as a basic reference and checklist, the new publication—Federal Information Processing Standards Publication (FIPS PUB) 64—is entitled *Guidelines for Documentation*

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of Computer Programs and Automated Data Systems for the Initiation Phase.

FIPS PUB 64 covers the documentation needed when objectives and requirements for new software are established. It includes a comprehensive listing of the elements of three basic initiation phase documents: project requests, feasibility study, and cost benefit analysis documents. Criteria to guide managers in selecting the right amount of documentation in planning and evaluating new software projects are also provided.

The recommended practices are for use by Federal agencies in documenting their data processing applications and are applicable to many different kinds of software. The time and effort spent in documentation can pay off in more cost-effective management and use of computer resources. Documentation provides the information needed by ADP managers and users in designing, operating, and maintaining software and in making software transportable to other users.

FIPS PUB 64 is designed to be used in conjunction with an earlier documentation guide issued by NBS, FIPS PUB 38, *Guidelines for Documentation of Computer Programs and Automated Data Systems*. This publication covers documentation practices for the development phase of the software life cycle.

Building Technology

Berry, S. A., Ed., *Proceedings of the National Conference on Regulatory Aspects of Building Rehabilitation*. Proceedings of a Conference held at the National Bureau of Standards, Gaithersburg, MD, Oct. 30, 1978, Nat. Bur. Stand. (U.S.), Spec. Publ. 549, 220 pages (Aug. 1979) Stock No. 003-003-20107-5, \$5.50.

Computer Science and Technology

Peacock, R. D., and Smith, J. M., *SPEED 2, A Computer Program for the Reduction of Data from Automatic Data Acquisition Systems*, Nat. Bur. Stand. (U.S.), Tech. Note 1108, 153 pages (Sept. 1979) Stock No. 003-003-02112-1, \$4.75.

Smid, M. E., *Computer Science and Technology: A Key Notarization System for Computer Networks*, Nat. Bur. Stand. (U.S.), Spec. Publ. 500-54, 35 pages (Oct. 1979) Stock No. 003-003-02130-0, \$1.75.

Wilson, C. B., *Computer Science and Technology: Technology Assessment: ADP Installation Performance Measurement and Reporting*, Nat. Bur. Stand. (U.S.), Spec. Publ. 500-53, 37 pages (Sept. 1979) Stock No. 003-003-02123-7, \$2.00.

Health and Safety

Sher, A. H., and Stenbakken, G. N., *Selection and Application Guide to Commercial Intrusion Alarm Systems*, Nat. Bur. Stand. (U.S.), Spec. Publ. 480-14, 40 pages (Aug. 1979) Stock No. 003-003-02098-2, \$4.00.

Energy Conservation and Production

Treado, S. J., Burch, D. M., and Hunt, C. M., *An Investigation of Air-Infiltration Characteristics and Mechanisms for a Townhouse*, Nat. Bur. Stand. (U.S.), Tech. Note 992, 36 pages (Aug. 1979) Stock No. 003-003-02090-7, \$3.50.

Engineering, Product and Information Standards

Reed, S. K., *Guideline for Automatic Data Processing Risk Analysis*, Nat. Bur. Stand. (U.S.), Fed. Info. Process. Stand. Publ. (FIPS PUB) 65, 27 pages (Aug. 1979).

Environmental Studies: Pollution Measurement

Becker, D. A., and Hurd, H. A., Eds., *Measurements and Standards for Recycled Oil—II*. Proceedings of a Conference held at the National Bureau of Standards, Gaithersburg, MD, Nov. 29-30, 1977, Nat. Bur. Stand. (U.S.), Spec. Publ. 556, 212 pages (Sept. 1979) Stock No. 003-003-02108-3, \$5.50.

Fire Research

Babrauskas, V., *Full-Scale Burning Behavior of Upholstered Chairs*, Nat. Bur. Stand. (U.S.), Tech. Note 1103, 86 pages (Aug. 1979) Stock No. 003-02110-5, \$3.50.

Rogers, G. J., and Evans, D. D., *Characterization of Electrical Ignition Sources Within Television Receivers*, Nat. Bur. Stand. (U.S.), Tech. Note 1109, 60 pages (Oct. 1979) Stock No. 003-02119-9, \$2.50.

Metrology: Physical Measurements

Souders, T. M., Flach, D. R., *A 20 Bit + Sign, Relay Switched D/A Converter*, Nat. Bur. Stand. (U.S.), Tech. Note 1105, 21 pages (Oct. 1979) Stock No. 003-003-02129-6, \$1.50.

Nuclear Physics and Radiation Technology

Heaton, H. T., II, and Jacobs, R., Eds., *Proceedings of a Conference on Neutrons from Electron Medical Accelerators*. Proceedings of a Conference held at the National Bureau of Standards, Gaithersburg, MD, Apr. 9-10, 1979, Nat. Bur. Stand. (U.S.), Spec. Publ. 554, 172 pages (Sept. 1979) Stock No. 003-003-02115-6, \$4.75.

Processing and Performance of Materials

Escalante, E., and Ito, S., *A Bibliography on the Corrosion and Protection of Steel in Concrete*, Nat. Bur. Stand. (U.S.), Spec. Publ. 550, 24 pages (Aug. 1979) Stock No. 003-003-02106-5, \$1.50.

Hastie, J. W., Ed., *Characterization of High Temperature Vapors and Gases*. Volumes 1 and 2. *Proceedings of the 10th Materials Research Symposium* held at the National Bureau of Standards, Gaithersburg, MD, Sept. 18-22, 1978, Nat. Bur. Stand. (U.S.), Spec. Publ. 561/1, 800 pages (Sept. 1979) Stock No. 003-003-02124-5, \$20.00.

Shives, T. R., and Willard, W. A., Eds., *MFPG—Advanced Composites: Design and Applications*. *Proceedings of the 29th Meeting of the Mechanical Failures Prevention Group*, held at the National Bureau of Standards, Gaithersburg, MD, May 23-25, 1979, Nat. Bur. Stand. (U.S.), Spec. Publ. 563, 304 pages (Oct. 1979) Stock No. 003-003-02120-2, \$7.00.

Standard Reference Materials

Marinenko, R. B., Heinrich, K. F. J., and Ruegg, F. C., *Standard Reference Materials: Micro-Homogeneity Studies of NBS Standard Reference Materials, NBS Research Materials, and Other Related Samples*, Nat. Bur. Stand. (U.S.), Spec. Publ. 260-65, 84 pages (Sept. 1979) Stock No. 003-003-02114-1, \$3.50.

Venable, W. H., Jr., and Eckerle, K. L., *Standard Reference Materials: Didymium Glass Filters for Calibrating the Wavelength Scale of Spectrophotometers—SRM 2009, 2013, and 2014*, Nat. Bur. Stand. (U.S.), Spec. Publ. 260-66, 85 pages (Oct. 1979) Stock No. 003-003-02127-0, \$3.50.

NEWS BRIEFS

NUCLEAR WASTE MANAGEMENT The NBS Office of Measurements for Nuclear Technology (OMNT) is formulating a major new program to study the measurement problems associated with nuclear waste management. The new program, to be instituted at the request of the Department of Energy, will develop measurement standards and techniques for nuclear wastes. The OMNT is the successor to the Office of Measurements for Nuclear Safeguards, which was created to coordinate Bureau research projects aimed at improving the accuracy with which nuclear materials are accounted for and controlled.

SMOKE DETECTORS IN MOBILE HOMES. In mobile homes, a properly functioning ionization or photoelectric smoke detector mounted near the ceiling on either the inside or the outside wall at the living room end of the corridor should provide an alarm in sufficient time to permit an alert and mobile occupant to escape in typical smoldering or flaming fires. That conclusion is based on a series of full-scale tests conducted by the NBS Center for Fire Research for the Department of Housing and Urban Development.

SURFACE PLANES STUDIED WITH FIELD ION MICROSCOPY. An NBS scientist, working in collaboration with two researchers from the University of Pennsylvania, is investigating the structure of crystal planes and their dependence on temperature using the field ion microscope. Preliminary data confirm that one of the major crystal planes of tungsten and molybdenum is indeed more complex than would be expected from the bulk structure, and that this difference occurs over a wider temperature range than had been known previously.

IMPROVED TECHNIQUE FOR DENSITY MEASUREMENT. Two NBS researchers have developed a simple new technique for measuring the density of solid objects with high precision. The researchers immerse both the weight and a top-loading electronic balance with servocontrol in a heavy fluorocarbon liquid normally used to cool power transformers. By making appropriate corrections for the change in density of the fluid, the researchers can make measurements without surface tension effects. Preliminary results indicate that measurements with a precision of up to a part in 10 000 can be made in no more than 15 minutes.

CORROSION BIBLIOGRAPHY A bibliographic list of 394 published papers, reports, and talks on the corrosion of steel in concrete and related subjects is now available. A subject index list references under six major subheadings: reviews, factors affecting corrosion, measurement techniques, protection techniques, concrete design, and related fields. A Bibliography on the Corrosion and Protection of Steel in Concrete (NBS Spec. Publ. 550) is for sale by the Superintendent of Documents, Washington, D.C. 20402, price \$1.50. Order by SD Catalog No. 003-003-02106-7.

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